POISSON EQUATION

Friday, 9 November 2018 09:05

$$\nabla \cdot (\varepsilon \nabla \phi) = -q \underbrace{\rho[\phi]}_{\text{density}}$$

charge density

$$\rho = [+p^{(\phi)} - n^{(\phi)} + N_D^+(\phi) - N_A^-(\phi)]$$

dielectric constant

$\phi(\vec{r})$ is the electrostatic potential from which you can extract the relevant information like CB and VB

PDE Partial Differential Equation

If we discretize (like what we have done for the Schrödinger equation) you get a problem like this:

$$M \phi = B[\phi]$$

If N_p is the number of the grid points

$$[N_p \times N_p]\,[N_p \times 1] = [N_p \times 1]$$

This problem is solved iteratively:

1 step:
- trial ϕ_1
- compute $\rho[\phi_1]$

  you solve
- $\nabla \cdot (\varepsilon \nabla \phi) = -q\rho[\phi_1]$ from this you get ϕ_2 out of $\phi_2 = M^{-1} \cdot q\rho[\phi_1]$

2 step:
- compute $\rho[\phi_2]$
- solve

  $\phi_3 = M^{-1} \cdot q\rho[\phi_2]$

⋮

if $\|\phi_{i+1} - \phi_i\| < \varepsilon$ then stop
else continue the iteration

self-consistent scheme

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"QUANTUM PHENOMENA" by S. DATTA

Whatever the confinement, the electronic charge can be expressed as:

$$n(\underline{r}) = \sum_{K} |\psi_K(r)|^2 \cdot f(E_K) \qquad f = \frac{1}{1 + \exp\left(\frac{E - E_F}{K_B T}\right)}$$

1D Confinement

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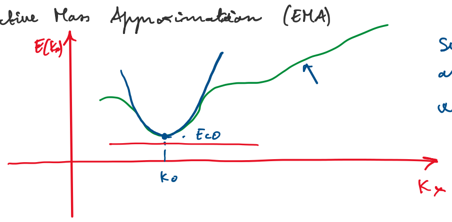
Let's suppose that the 1D confinement is on the x-direction

The eigenfunction can be expressed as:

$$\Psi_{i,k_y,k_z}(x,y,z) = \varphi_i(x,y,z)\,\frac{e^{jk_y y}}{\sqrt{L_y}}\cdot\frac{e^{jk_z z}}{\sqrt{L_z}}$$

$$n(x,y,z) = \sum_{i,k_y,k_z} |\Psi_{i,k_y,k_z}|^2 f(E_{i,k_y,k_z})$$

E_{i,k_y,k_z} is the energy dispersion, which is approximated through Effective Mass Approximation (EMA)



Since we are interested only at bottom of the conduction band, we approximate the E(k) with a parabola.

$$E(k) \simeq E_{c0} + \underbrace{\frac{\delta E}{\delta k}(k-k_0)}_{=0} + \underbrace{\frac{1}{2}\frac{\delta E}{\delta k^2}(k-k_0)^2}_{\frac{\hbar^2}{2m_x}}$$

At the bottom of the E(k)

$$E(k) \simeq E_{k0} + \frac{1}{2}\frac{\hbar^2}{m_x}(k-k_0)^2 \longrightarrow m_x = \frac{\hbar^2}{\left(\frac{\delta^2 E}{\delta k^2}\right)}$$

So, in the EMA, E_{i,k_y,k_z} can be expressed as:

$$E_{i,k_y,k_z} = \underbrace{\mathcal{E}_i}_{\substack{\text{discrete eigenvalue}\\ \text{coming from the}\\ \text{1D Schrödinger equation (within EMA well)}}} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z} \Big\} \text{ 2D subband}$$

$$n(x,y,z) = \sum_i \sigma_i |\varphi_i(x,y,z)|^2, \text{ where } \sigma_i \triangleq \sum_{k_y,k_z}\frac{f(E_{i,k_y,k_z})}{L_y L_z}$$

$$\sum_{k_y,k_z} \longrightarrow \frac{2L_yL_z}{(2\pi)^2}\int d^2k$$

$$\boxed{k_y' = \frac{k_y}{\sqrt{2m_y}}\;;\quad k_z' = \frac{k_z}{\sqrt{2m_z}}}$$

Change of variables

$$d^2k = dk_y\,dk_z = 2\sqrt{m_y m_z}\,dk_y'\,dk_z'$$

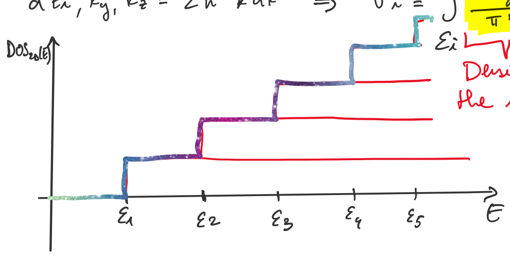
$$E_{i,k_y',k_z'} = \mathcal{E}_i + \hbar^2 k_y'^2 + \hbar^2 k_z'^2 = \mathcal{E}_i + \hbar^2 k'^2 \qquad \boxed{k'^2 = k_y'^2 + k_z'^2}$$

Let's change the coordinate system:

$$d^2k = k\,dk\,d\vartheta, \text{ so the integral becomes: } \frac{\cancel{2}L_yL_z}{\cancel{4}\pi^2}\,\cancel{2}\sqrt{m_y m_z}\int_0^{2\pi}d\vartheta\int_0^{+\infty}k'dk'$$

$$\sigma_i = \int_0^{2\pi}d\vartheta\int_0^{+\infty}\frac{\sqrt{m_y m_z}}{\pi^2}k'dk'\,f(E_i,k_y',k_z') = 2\cancel{\pi}\int_0^{+\infty}\frac{\sqrt{m_y m_z}}{\pi\cancel{^2}}k'dk'\,f(E_i,k_y',k_z')$$

$$dE_i,k_y,k_z = 2\hbar^2 k'dk' \Rightarrow \sigma_i = \int_{\mathcal{E}_i}^{+\infty}\underbrace{\frac{\sqrt{m_y m_z}}{\pi\hbar^2}}_{\substack{\text{Density of states of}\\ \text{the } i\text{-th 2D subband}}} f(E_i,k_y,k_z)\,dE_{i,k_y,k_z}$$



$$\sigma_i = \frac{\sqrt{m_y m_z}}{\pi\hbar^2}k_BT\ln\left[1+\exp\left(-\frac{\mathcal{E}_i - E_F}{k_BT}\right)\right]$$

$$\boxed{n_{2DEG} = \sum_i |\varphi_i|^2\frac{\sqrt{m_y m_z}}{\pi\hbar^2}k_BT\ln\left[1+\exp\left(-\frac{\mathcal{E}_i - E_F}{k_BT}\right)\right]}$$

2D confinement

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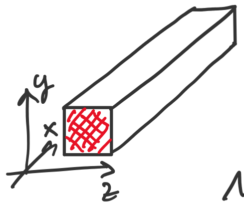
$$\psi_{k_x,i} = \frac{e^{jk_x x}}{\sqrt{L_x}}\chi_i(y,z) \;;\quad E_{i,k_x} = \mathcal{E}_i(x) + \frac{\hbar^2 k_x^2}{2m_x}$$



confined along the y-z plane

$$n(x,y,z) = \sum_i |\chi_i|^2 \alpha_i$$

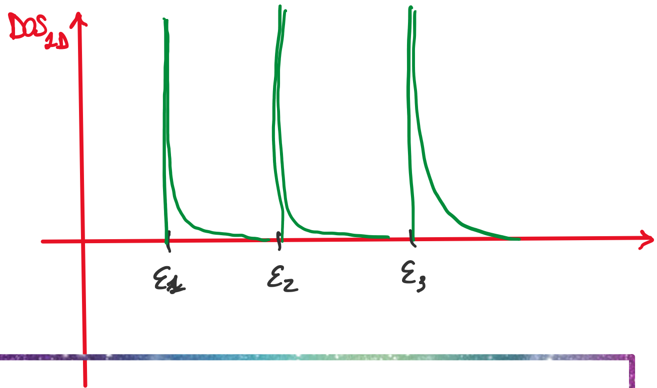
$$\alpha_i \triangleq \sum_{k_x} \frac{f(E_{i,k_x})}{L_x}$$

$$\alpha_i = \frac{2\cancel{L_x}}{2\pi}\int_{-\infty}^{+\infty}\frac{f(E_i,k_x)}{\cancel{L_x}}\,dk_x = \frac{2}{\pi}\int_{0}^{+\infty} f(E_i,k_x)$$ since f is a pair function

Since

$$k_x = \frac{\sqrt{2m_x(E-\mathcal{E}_i)}}{\hbar} \Rightarrow dk_x = \frac{\sqrt{2m_x}}{2\hbar\sqrt{E-\mathcal{E}_i}}\,dE$$

$$\alpha_i = \int_{\mathcal{E}_i}^{+\infty} \underbrace{\frac{2m_x}{\pi\hbar}\frac{1}{\sqrt{E-\mathcal{E}_i}}}_{DOS_{1D}} f(E-\mathcal{E}_i)\,dE$$



FERMI-DIRAC INTEGRALS

$$F_j(x) = \frac{1}{\Gamma(j+1)}\int_0^{+\infty}\frac{t^j}{e^{t-x}+1}\,dt$$

$$\frac{\partial F_j}{\partial x} = F_{j-1}$$

see: "NOTES ON FERMI-DIRAC INTEGRALS"
R. KIM & M. LUNDSTROM

$$F_{-\frac{1}{2}}(y) = \int_0^{+\infty}\frac{1}{\sqrt{x}}\,\frac{1}{1+\exp(x-y)}\,dy$$

$$\boxed{n_{1D} = \frac{1}{\pi}\left(\frac{2m_x k_B T}{\hbar^2}\right)^{1/2}\sum_i |\chi_i|^2 F_{-\frac{1}{2}}\left(\frac{E_F-\mathcal{E}_i}{k_B T}\right)}$$

3D Confinement

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$$n = \sum_i |\psi_i|^2 \frac{1}{1+\exp\left(\frac{E_i - E_F}{k_B T}\right)}$$